Stability of the photonic band gap in the presence of disorder

M. A. Kaliteevski,[1,*] D. M. Beggs,[1] S. Brand,[1] R. A. Abram,[1] and V. V. Nikolaev[2]
[1]*Department of Physics, University of Durham, Durham, DH1 3LE, United Kingdom*
[2]*Ioffe Physicotechnical Institute, 26, Polytechnicheskaya, St-Petersburg, Russia*
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The photonic eigenmodes near a band gap of a type of one-dimensional disordered photonic crystal have been investigated statistically. For the system considered, it is found that the tail of the density of states entering the band gap is characterized by a certain penetration depth, which is proportional to the disorder parameter. A quantitative relation between the relative penetration depth, the relative width of the photonic band gap, and the disorder has been found. It is apparent that there is a certain level of disorder below which the probability of the appearance of photonic eigenstates at the center of the photonic band gap essentially vanishes. Below the threshold, the ensemble-averaged transmission at the center of the photonic band gap does not change significantly with increasing disorder, but above threshold it increases much more rapidly. A simple empirical formula has been obtained which describes how the logarithm of the transmission relates to the periodic refractive index modulation and the disorder.

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At present it is impossible to produce an ideal photonic crystal for use at optical wavelengths. The deviation of the sphere diameters in opals[1] and the roughness of the walls in lithographically produced structures lead to departures from the intended periodic spatial distribution of dielectric constant.[2] Such imperfections can damage the photonic band gap (PBG) significantly and result in a finite value of the density of states across the whole of the intended gap.[3] As a result, much effort has been spent on investigations of the influence of disorder on the PBG and the related problem of wave localization in disordered optical media, which is called Anderson localization in analogy with electron localization.[4]

As has previously been pointed out[5] the term localization is commonly viewed in different ways in different areas of physics. For example, in quantum mechanics particle localization is usually discussed in terms of the existence of solutions of the Schrödinger wave equation which decay exponentially from a certain region of space,[6] while in optics it is more natural to consider the propagation of light, and total reflection from a disordered medium is taken to be indicative of photonic localization.[5,7]

Nevertheless in an infinite one-dimensional (1D) disordered photonic system, each state is localized in the sense that the density of electromagnetic energy $\varepsilon(z)$ (or equivalently probability density in the particle case) has the form $\lim_{z\to\infty}\varepsilon_i(z)\sim\exp(-|z|/\gamma_i)$ where z is the position relative to the region of localization.[6,8,9] No definite conclusion about system behavior can be made for limited values of $|z|$ but a consequence of such localization is that for a finite disordered system the transmission coefficient averaged over an ensemble of structures $\langle T\rangle$ decays exponentially with increasing system size L, and can be described by an attenuation length ξ through the relation $\langle\ln(T)\rangle\sim -L/\xi$. However, it is important to realize that similar transmission properties can be observed in perfectly ordered systems—photonic crystals—if the frequency corresponds to the photonic band gap (PBG). In this case the exponential decay is described by the imaginary part of the Bloch wave vector. A distinction between the two phenomena is that the localization length for Anderson localization decreases with increasing disorder, while for photonic crystals at frequencies corresponding to a PBG, ξ grows with increasing disorder.[10]

There have been numerous attempts to apply scaling theory in the analysis of localization in disordered photonic crystals.[11] However Deych *et al.*[12] have demonstrated anomalous behaviour of the variance of the Lyapunov exponent ξ^{-1} and concluded that although states at frequencies corresponding to bands of the photonic crystal have regular Anderson behavior, there are gap states that do not. They have also shown that there is a critical value of disorder, above which the anomalous behavior of the Lyapunov exponent disappears and all the states exhibit normal Anderson-like behaviour. Therefore the exponential dependence of the ensemble-averaged transmission coefficient on the length of the structure does not allow us to make any definite conclusions about the modal structure of electromagnetic field.

In 1987 John stated that the "photonic band gap is filled with localized photonic states even in the case of weak disorder,"[13] but no quantitative estimate of the density of states or other characteristics of the gap states were provided. However, in 1999 Vlasov and co authors[10] found that as long as the disorder does not exceed a certain threshold value, the attenuation length within the PBG does not change significantly with increasing disorder. As a result, they suggested that, in contrast to John's statement, localized states do not appear in the PBG for disorder below threshold, but they did not demonstrate that explicitly by calculating the mode spectrum.

Therefore, in an effort to clarify the physical picture of light localization in disordered photonic crystals we have conducted *ab initio* calculations of both the mode structure of the electromagnetic field and the photon transport properties of 1D disordered photonic crystals.

We consider a one-dimensional periodic structure, which is a sequence of a pair of layers A and B of the same thickness $D/2$, whose refractive indices are $n_{A,B}^{(0)}=n_0\pm g$ where g is the modulation of the refractive index, and n_0 is the average refractive index. An infinite structure possesses PBGs, whose positions can be determined by solving the dispersion equation $2\cos(KD)=\mathrm{tr}[\hat{\mathbf{T}}(\omega)]$, where K is the Bloch wave vector and $\hat{\mathbf{T}}$ is the transfer matrix for one period. The center of the first PBG is at $\omega_0 = \pi c/n_0 D$, and the relative width of the gap is $\Delta\omega/\omega_0 \approx 4g/\pi n_0$. In the case of a structure of finite size, the mode spectrum is discrete and the eigenfrequencies can be obtained by setting outgoing wave boundary conditions, corresponding to light not being incident on the structure, using the equation

$$A\begin{pmatrix} 1 \\ -n_f \end{pmatrix} = \hat{\mathbf{M}}\begin{pmatrix} 1 \\ n_l \end{pmatrix}. \tag{1}$$

Here n_f and n_l are the refractive indices of the semi-infinite media surrounding the structure, $\hat{\mathbf{M}}$ is the transfer matrix through the whole structure, and A is a constant. Note that the frequencies of the eigenmodes ω_i will have nonzero imaginary parts, due to the leakage of the light through the boundaries. In other words, the lifetime of the eigenmodes $\tau = 1/\mathrm{Im}(\omega_i)$ will be finite. By analyzing the value of the lifetime, one can conclude whether the mode is localized or not, according to the Thouless criterion.[14] For electrons the Thouless criterion considers a state to be localized if the width of the energy level (proportional to the inverse lifetime) is less than the separation of energy levels; otherwise the state is extended.

The squares in Fig. 1 denote the frequencies and lifetimes of the states in an ideal periodic structure of the length $L = 200D$ with $n_0 = 2$ and $g = 0.025$, surrounded by semi-infinite media with refractive indices $n_f = n_l = 1$. An infinite structure with such parameters possesses a PBG of relative width $\Delta\omega/\omega_0 \approx 0.016$, whose boundaries are shown by vertical lines in Fig. 1. The lower horizontal line in each plot gives the lifetime of the modes in the structure for which $g = 0$ (i.e., the Fabry-Pérot modes of a uniform structure). For these modes the inverse lifetime is comparable to the frequency interval between modes, and such states are delocalized. Periodic modulation of the refractive index leads to an increase of the lifetime of the eigenmodes, and the increase is more pronounced for the states close to the PBG edges. The states closest to the edge of the PBG are called edge states, and were first described by Kogelnick and Shank[15] in the context of distributed feedback lasers. According to the Thouless criterion the edge states are localized, but the density of electromagnetic energy decays to the edges of the structure more slowly than exponential.

For the study of the properties of disordered structures we introduce random fluctuations of the refractive indices: for each pair of layers A and B in the unit cell, the refractive indices are defined by the formula $n_{A,B} = n_0 \pm g + n_0 \delta P$, where P takes random values in the interval from $-\frac{1}{2}$ to $\frac{1}{2}$ and δ is constant for a particular structure that specifies the level of disorder. Thus the optical lengths D_i of the unit cells in a particular disordered structure are given by

$$D_i = D(n_A + n_B)/2 = Dn_0(1 + \delta P) = D_0(1 + \delta P), \tag{2}$$

where $D_0 = n_0 D$ and the range of the random fluctuations in D_i/D_0 is given by δ.

The dots in Fig. 1 represent the solutions of Eq. (1) and are plotted as $[\mathrm{Re}(\omega_i), 1/\mathrm{Im}(\omega_i)]$ for 10^3 disordered structures with different configurations of the disorder characterized by the value of δ. For $\delta = 0.035$, the eigenfrequencies $\mathrm{Re}(\omega_i)$ and their lifetimes τ fluctuate near the values corresponding to the eigenmodes of the ideal structure, but the fluctuations of the lifetime of the edge states near the PBG are larger than for those further away. Some of the modes penetrate into the PBG but there is no qualitative change of mode spectrum, as illustrated in Fig. 2, where the density of states (DOS) averaged over an ensemble of 10^4 structures is shown by circles. The fluctuation of D_i can also be obtained by varying the layer thicknesses as described above for the refractive index, and for this case the resulting DOS is shown by squares in Fig. 2.

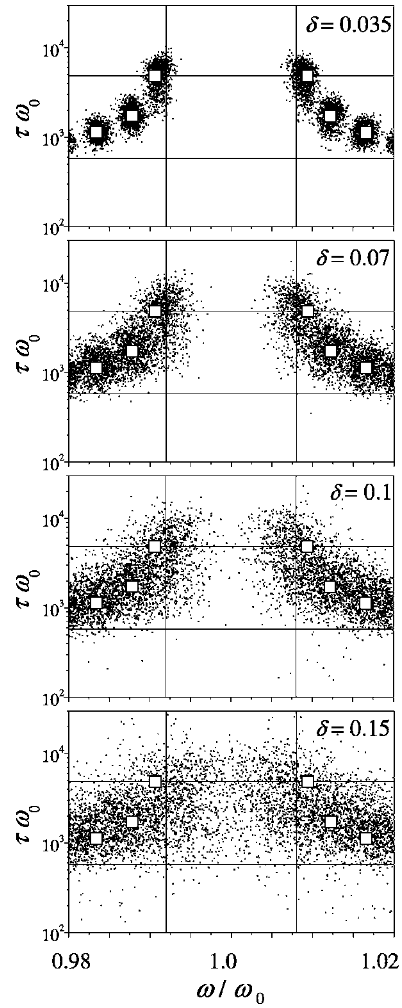

FIG. 1. White squares denote the frequencies $\mathrm{Re}(\omega_i)$ and lifetimes $\tau = 1/\mathrm{Im}(\omega_i)$ for an ideal structure ($\delta = 0$). Dots show frequencies and lifetimes for eigenmodes obtained by solving Eq. (1) for 10^3 disordered structures with $\delta = 0.035$, 0.07, 0.1, and 0.15. The thickness of the structure is $L = 200D$ and the modulation of refractive index is $g = 0.025$.

When the refractive indices and thicknesses of the layers are taken to fluctuate simultaneously and independently, and the fluctuation of each quantity is characterized by a top-hat distribution of relative width δ, the distribution function of the optical length D_i of a period of the structure will be almost a Gaussian with width close to δ, as shown in the inset to Fig. 2 by the dotted line. The resulting DOS is shown in Fig. 2 by stars. Note that due to similar widths of the top-hat and Gaussian distributions of D_i, the densities of states are practically identical for all the types of disorder

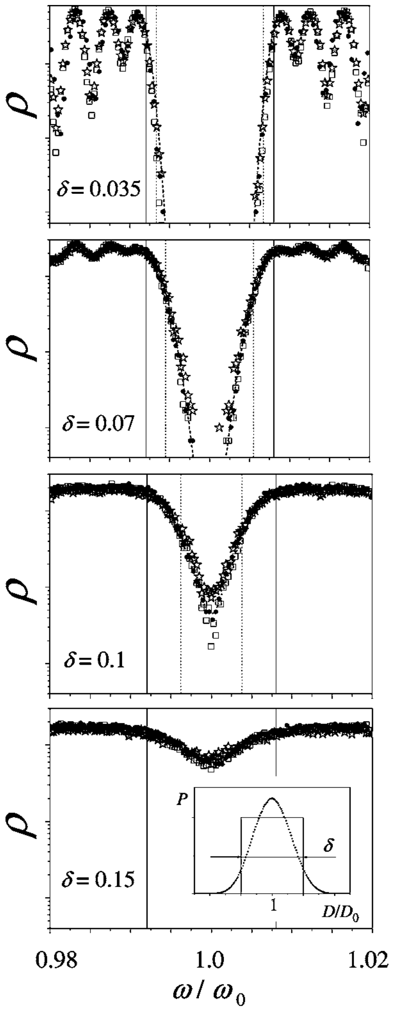

FIG. 2. Density of states averaged over ensembles of 10^4 structures with δ=0.035, 0.07, 0.1, and 0.15, plotted on a logarithmic scale. Circles (squares) correspond to the case of fluctuation of the optical length of the periods D_i with a square distribution function, shown in the inset of the lower graph by the solid line, due to fluctuations of the refractive indices (widths) of the layers. Stars correspond to the near Guassian distribution of D_i shown in the inset by the dotted line. Vertical solid lines show the boundaries of the PBG for the ideal structure. Dashed lines show the fit for the density of states within the PBG using Eq. (3). Vertical dotted lines indicate the penetration depth Ω for each case.

considered. Thus we conclude that the density of modes in a disordered photonic crystal is defined by the relative fluctuation of the optical length of one period of the structure.

The shape of the tails in the density of modes within the PBG is described with very high accuracy by the formula

$$\rho \sim \exp\left(-\frac{(\omega-\omega_e)^2}{\Omega^2}\right), \tag{3}$$

where ω_e is the angular frequency of the relevant band edge in the crystal and Ω is penetration depth. The penetration depth Ω is found to be proportional to δ but does not depend on the length of the structure (as is to be expected since the density of states is a self-averaging quantity).

When δ is increased to 0.07, the edge states penetrate further into the PBG and the fluctuations of the lifetime of the modes increase. The width of the PBG is reduced but nevertheless remains substantial. Eventually, when δ is increased to 0.1, the probability of the appearance of eigenmodes in any part of the original PBG becomes substantial and the fluctuations in the lifetimes of the eigenstates are greater.

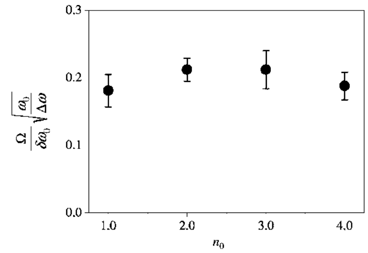

FIG. 3. The quantity $(\Omega/\delta\omega_0)\sqrt{\omega_0/\Delta\omega}$ for structures characterized by different values of the average refractive index n_0. The vertical bars indicate the standard deviation of this quantity. 10^4 structures were modeled for each set of the parameters n_0, g, and δ. The parameters g and δ are varied over the ranges 0.0125 to 0.125 and 0.01 to 0.2 respectively.

An increase of δ to 0.15 leads to a decrease in the dip of the density of states, an increase of the fluctuations of the lifetime, and a slight decrease of its mean value. Further increase of δ leads to the disappearance of the effects associated with the periodic modulation of the refractive index, and the system becomes completely disordered. We believe that the filling of the PBG with states is the reason for the transition from anomalous to normal behavior of the Lyapunov exponent observed in Deych *et al.*[12]

For all the structures considered, the penetration depth Ω is proportional to the square root of the relative band gap width $\Delta\omega/\omega_0$.

In Fig. 3 the dimensionless quantity $(\Omega/\delta\omega_0)\sqrt{\omega_0/\Delta\omega}$ is plotted as a function of the average refractive index in the structure n_0 which is related to the frequency of the center of the PBG. The plot leads us to conclude that the penetration depth is decribed by the formula

$$\frac{\Omega}{\omega_0} \approx \frac{\delta}{5}\sqrt{\frac{\Delta\omega}{\omega_0}}, \tag{4}$$

i.e., the relative penetration depth exhibits a universal dependence on the relative gap width.

Equation (4) provides a means to specify a practical criterion for the resilience of the PBG to the presence of disorder. Assuming that for a particular application there is a certain acceptable level of the density of states at the center of the gap described by a suppression factor S_{th}, which is defined as the ratio of the densities of states at the center and the edge of the PBG, the threshold value of the disorder δ_{th} is

$$\delta_{th} \approx \frac{5}{2\sqrt{-\ln S_{th}}}\sqrt{\frac{\Delta\omega}{\omega_0}}. \tag{5}$$

For example, suppression of the density of states at the center of the PBG by a factor 10^{-8} would correspond to $\Omega \approx \Delta\omega/9$, and a threshold disorder parameter given by $\delta_{th} \approx \sqrt{(\Delta\omega/\omega_0)}/3$. Note that the square root of the logarithm in Eq. (5) varies very slowly with the change of the argument,

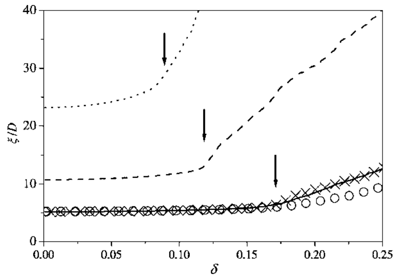

FIG. 4. Dependence of the attenuation length ξ at the center of the PBG on the disorder parameter δ for structures with modulation of that of the refractive index $g=0.025$ (dotted line); $g=0.05$ (dashed line); $g=0.1$ (solid line). Symbols show the dependences obtained for the case by the transformation ($\xi \to \xi/\alpha$, $\delta \to \delta\sqrt{\alpha}$) of the results for the structures with $g=0.025$ (circles) and $g=0.05$ (squares). Here α is the ratio of the attenuation lengths for the structures with $g=0.025$ or $g=0.05$ and the attenuation length for the structure with $g=0.1$. Arrows indicate the threshold values of δ. The thickness of the structure is $L=200D$.

and the above estimate can be considered as an almost universal criterion for the stability of the PBG in one-dimensional photonic crystals in the presence of disorder.

At the center of the PBG, the transmission coefficient decays exponentially with the increase of the structure length. The dependence of the attenuation length ξ, defined as $\xi=-L/\ln\langle T\rangle$, on the fluctuation parameter δ for structures with $g=0.025$, $g=0.05$, and $g=0.1$ is shown in Fig. 4. For all the cases considered, the dependences are characterized by a threshold; when $\delta<\delta_{th}$, ξ grows very slowly with increasing δ, and the attenuation length ξ is virtually unchanged. When δ reaches δ_{th}, a threshold occurs in the dependence of ξ on δ, and ξ grows much faster with increasing δ. Such behavior can be easily explained. The increase of $\langle T\rangle$, and hence ξ is a consequence of the appearance of sharp spikes, corresponding to localized eigenmodes in the transmission spectrum of individual structures.[10] When $\delta<\delta_{th}$, the increase of the transmission coefficient is provided by the tails of such spikes and therefore is very small. When $\delta>\delta_{th}$, localized states and corresponding peaks in transmission spectra can appear in the center of the PBG, and $\langle T\rangle$ starts to grow faster with increasing δ.

The dependence of δ_{th} on the relative width of the PBG (or on the attenuation length ξ_0 in the ideal structure) in Eq. (5) has an interesting consequence. If $\alpha=g^{(1)}/g^{(2)}$ is the ratio of modulations of the refractive indices $g^{(1)}$ and $g^{(2)}$ for two ideal structures, then the dependences of the attenuation length ξ on δ for the two structures are coupled remarkably well by the relation

$$\alpha\xi^{(1)}(\delta) = \xi^{(2)}(\delta\sqrt{\alpha}). \tag{6}$$

In Fig. 4 the crosses show the result of the transformation (6) on $\xi(\delta)$ for the structure with $g=0.05$, when $\alpha=\xi_0(g=0.05)/\xi_0(g=0.1)$. The circles show the result of the corresponding transformation for the structure with $g=0.025$, and $\alpha=\xi_0(g=0.025)/\xi_0(g=0.1)$. For the structures with $g=0.025$ and $g=0.1$, the transformation (6) couples the dependences $\xi(\delta)$ with very high accuracy. For the structure with $g=0.025$, when δ is larger than the threshold value, some deviation occurs at the higher values of δ due to the fact that the attenuation length is comparable to the sample size, and the influence of boundaries is substantial.

The transformation in Eq. (6) reflects a universal behavior of the attenuation length (and transmission coefficient) in disordered photonic crystals, and could be useful in the development of analytical theories of such systems. Finally we note that the thresholdlike behavior of a transmission coefficient on the disorder parameter has also been demonstrated for two-dimensional photonic crystals.[16,17]

To conclude, we have analyzed quantitatively the penetration of states into the band gap of a type of one-dimensional disordered photonic crystal. We have shown that the tail of the density of states in the band gap has a Gaussian form characterized by a penetration depth parameter and there is an allowed level of disorder below which the probability of the appearance of photonic eigenstates at the center of photonic band gap essentially vanishes. A relationship between the relative penetration depth, relative gap width, and disorder parameter has been found and a scaling formula relating the attenuation length to the gap width and disorder has also been obtained.

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*Email address: m.a.kaliteevski@durham.ac.uk

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